PyCUDA: GPU Run-Time Code Generation for High-Performance Computing

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Abstract

High-performance scientific computing has recently seen a surge of interest in heterogeneous systems, with an emphasis on modern Graphics Processing Units (GPUs). These devices offer tremendous potential for performance and efficiency in important large-scale applications of computational science. However, exploiting this potential can be challenging, as one must adapt to the specialized and rapidly evolving computing environment currently exhibited by GPUs. One way of addressing this challenge is to embrace better techniques and develop tools tailored to their needs. This article presents one simple technique, GPU run-time code generation (RTCG), and PyCUDA, an open-source toolkit that supports this technique.

In introducing PyCUDA, this article proposes the combination of a dynamic, high-level scripting language with the massive performance of a GPU as a compelling two-tiered computing platform, potentially offering significant performance and productivity advantages over conventional single-tier, static systems. It is further observed that, compared to competing techniques, the effort required to create codes using run-time code generation with PyCUDA grows more gently in response to growing needs. The concept of RTCG is simple and easily implemented using existing, robust tools. Nonetheless it is powerful enough to support (and encourage) the creation of custom application-specific tools by its users. The premise of the paper is illustrated by a wide range of examples where the technique has been applied with considerable success.

Key words: GPU, Many-core, Code generation, Automated Tuning, Software engineering, High-level Languages, Massive Parallelism, Single-instruction multiple-data

1. Introduction

Graphics Processing Units (GPUs)\textsuperscript{7, 23, 34} promise tremendous advantages in throughput over conventional processor architectures, ideally resulting in a large reduction of execution time for suitable compute- or bandwidth-bound algorithms. However, execution time is not the only time scale to consider when comparing computer architectures. Indeed, the development time for a scientific code will, in many cases, be a significant fraction of its useful lifespan. GPUs now threaten to tip this balance even further out of the programmer’s favor, through the following four factors.

First, there is still much change going on in the area of massively parallel processors. These changes are driven by many factors–chip manufacturing processes change, new ideas and abstractions in hardware and software emerge and disappear at a rapid pace, market conditions change. Programs that work well on last year’s machines may not continue to represent optimal choices today. While the recent ratification of

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the OpenCL standard \cite{OpenCL} may bring a moment of stability, the landscape of devices that may be accessed is still large and ever-changing. Even though some patterns are emerging, the world is still very far from having settled on a programming model for massively parallel machines—a model that is as stable as the one we have enjoyed on CPUs for the last few decades.

Second, GPU code is very sensitive to seemingly innocent changes. Hardware implementation details are much more visible and have a much greater performance effect in GPU programs than they do in today’s CPU programs. Relative component clock rates, bus widths, vector widths, memory and buffer sizes all have an immediate impact on a successful code. The very premise of GPU computing is to try and find a better use for the silicon tied up in the caching, speculation and out-of-order execution that frees a modern CPU developer from having to worry about hardware peculiarities. We therefore expect that GPU developers will continue to be exposed to these details.

Third, and potentially a corollary of the last point, GPUs offer many more implementation choices, and often little guidance on which choice may lead to efficient code. It is not uncommon to see differences of an order of magnitude in execution time between codes that accomplish the same basic task. This is not likely to occur on a current-generation CPU, where, with few exceptions, “reasonably coded” and “highly optimized” fall within at most a factor of two or three of each other.

The fourth and possibly worst factor is that GPU development tools are in their infancy. Many years have been spent creating development tools that help the CPU developer achieve high productivity. These tools range from high-level languages and libraries that allow the programmer to deal in convenient abstractions, to optimizing compilers, debuggers, and profilers, which likewise shield the programmer from having to deal with the full complexity of the hardware. Many of these tools are either unavailable, inadequate or rudimentary on today’s parallel architectures.

We propose that GPU run-time code generation (“RTCG”) helps the programmer reclaim a significant share of the productivity lost to these factors. By GPU RTCG, we mean the ability to seamlessly execute arbitrary, generated low-level C (or C-like) source code for high-volume computational tasks in the context of the generating program. In the form described in this paper, the generation and execution of the low-level code is performed from a high-level scripting language. By the term “scripting language” or “high-level language”, we mean a language that

- enables various programming paradigms (e.g. functional, procedural, object, aspect, etc.),
- is dynamically typed,
- includes error reporting facilities,
- manages resources automatically,
- offers comprehensive built-in functionality,
- requires no user-visible compilation (i.e. suitable for interactive use), and
- works well as a “glue language” for lower level building blocks.

The family of major general-purpose scripting languages at the time of this writing includes Python, Ruby, Lua, and JavaScript and numerous others.

The present work describes lessons learned from many earlier approaches. GPU RTCG is a form of “metaprogramming”: instead of directing computer code immediately at a problem, one directs code at the creation of and reasoning about another piece of code which then solves the problem at hand. It is not initially clear that this additional level actually results in any tangible gain, but we defer this discussion to the later parts of this article. For now, it should suffice to say that we are by no means the first to apply the basic principle. Today, perhaps the most common mechanism used to implement metaprogramming ideas is the template mechanism of the C++ programming language. Many things have been implemented in this effective (if cumbersome) way: Expression evaluators \cite{expression_eval}, parser generators \cite{parser_generator}, even entire PDE solver frameworks \cite{pde_solver_framework}. The template-based technique is however constrained to being applied at the time when
the software is built, which limits its usefulness. A variety of ways have been devised to circumvent this restriction, reaching from assembly of small prefabricated pieces into a full code [9], to build-time evaluation of different code versions [44]. It should further not be forgotten that the Lisp programming language already brought the fundamental insight of the von Neumann architecture, namely that ‘code is data’, to higher-level languages in the early 1960s [24], albeit not necessarily with computational efficiency as the primary target.

In the context of GPUs, metaprogramming has so far been applied mainly in a graphics and image processing context [21, 43] and to ease the use of a standard rendering pipeline for general-purpose uses [36]. Other projects focus on generating GPU code using a compile-time C++-based framework [26, 25].

Further, this work can be seen in the context of recent efforts [22] to promote program generation as a mainstream idea. In comparison however, we are choosing a decidedly simple approach that values pragmatism over theoretical appeal: Why should we invent new tools from scratch when good results are achievable using a scripting language with a GPU and a C compiler? Curiously, many previous authors give up the immeasurable advantage of being able to generate code at run time all too easily. This capability is the main point of this article.

The text is organized as follows: We begin by giving a very brief overview of how GPUs differ from other computing platforms, first from the point of view of hardware in Section 2 then from that of software in Section 3. We continue in Section 4 by providing a sampling of problems arising from a GPU’s special structure where GPU RTCG can be profitably applied. Section 5 then describes a scripting-based approach to these problems that is supported by our open-source PyCUDA toolkit. Section 6 describes how a number of applications from varied disciplines have benefited from the approach in general and PyCUDA in particular. Finally, in Section 7 we close with a few remarks and ideas for future work.

2. GPU Hardware: A Brief Introduction

In the early days of GPU programming, the programmer had to repurpose marginally programmable fixed-function graphics hardware for computing purposes by a variety of methods [29]. With today’s generation of GPUs, this is not true any more. Instead, GPUs should be viewed as general-purpose floating point processors that are designed for a different type of target workload than current CPUs, and “GPU” becomes just a convenient moniker for this type of technology. For CPUs, the set of design workloads typically includes web browsers, word processors and a diverse collection of other desktop programs—characterized by high complexity and marginal potential for parallelization. GPUs, on the other hand, are aimed at applying uniform, moderately complex floating point operations to large volumes of data (i.e. “stream processing” [41]).

One of the most significant problems that modern processor design needs to address is the slowness of memory. While there have been significant advances in latency and access speed to affordable, large-scale, off-chip random access memory, these advances have in no way kept pace with the progress made in the throughput of processor cores. Variants of Moore’s Law predicted this latter progress to be exponential in nature, and so far reality has kept pace with prediction. This pace was not matched by the development of dynamic RAM (DRAM), the presently dominant technology for such memory. Therefore, the time between the issuing of a memory request by a core and the subsequent response from off-chip memory can be very long, measured in processor timescales.
While bandwidth can be increased to some extent by widening and improving the memory interface, latency cannot, as it is a fundamental property of the type of memory. Obviously, the design workloads for CPUs are very vulnerable to memory delays, and therefore CPU designers tend to take extreme measures to mitigate their effects. Three types of strategies are particularly popular here: First, include large amounts of fast cache memory on the chip to avoid having to wait for off-chip memory at all. Second, engage in many forms of prediction and speculation to make sure that required data is already present on-chip when it is needed. And finally, reorder the instruction stream to lessen the impact of memory-related stalls.

It is apparent that the hardware implementation of all these strategies can easily occupy large amounts of silicon. In contrast, the target workloads for a GPU are much less vulnerable to memory-related stalls. Since GPUs aim to apply similar operations to large amounts of data, exact ordering is less important. This allows the use of a much larger number of execution contexts, each of which may occupy a functional (i.e. floating-point or integer) unit whenever it has data available. While the management of large numbers of contexts is nontrivial in itself, the associated management logic is less expensive to implement than the CPU’s strategies, freeing a GPU to dedicate much more chip space to functional units, further increasing parallelism.

This abundance of functional units confronts GPU designers with yet another interesting challenge. Context management logic grows strongly superlinearly with the number of contexts it manages. One set of central logic that would manage the execution of all contexts on all functional units on the chip would be prohibitively large. This, together with physical limits of on-chip signal propagation speed, strongly suggests dividing up the available chip are into individual sub-processors, each of which manages a more limited set of execution contexts. It is the same thinking that drives heavyweight CPUs towards integrating multiple cores on a single die. Likewise, modern GPUs contain tens of management subdomains, each of which may manage hundreds of execution contexts. (These subdomains are called ‘compute units’ by OpenCL, ‘multiprocessors’ by Nvidia, and simply ‘cores’ by others. Execution contexts are called ‘threads’ by Nvidia and ‘work items’ by OpenCL.) To further improve the functional-unit-to-control-logic ratio and reach the cited width of hundreds of contexts per subdomain, most GPUs are built as relatively wide SIMD (Single Instruction Multiple Data) vector machines.

The chip→unit→context hierarchy has a twofold effect on GPU software: First, each unit is typically designed to operate independently of its siblings, limiting communication to contexts executing on the same unit. Second, programs must explicitly specify how to use each level of parallelism, typically by providing a suitable decomposition of an index space. Together with the remaining possibility of sequential execution, this poses the problem of loop slicing. Given a sequential description of the algorithm as a set of nested loops, loop slicing refers to the combined process of

- identifying loop axes that can serve as parallelization indices,
- assigning loop axes to available parallelization axes, such as compute units, execution context numbers within a unit, and SIMD lanes,
- interchanging loop orders to achieve a more beneficial order of memory accesses, and lastly,
- finding size restrictions on each loop axis, and splitting axes as necessary.

Observe that each of the above steps may depend on the outcome of all the others, resulting in a complicated joint optimization problem. The purpose of the remainder of this article is to explore these (and other) software challenges and propose solutions for some of them.

3. GPU Software Creation

In the preceding sections, we have already argued that software for GPUs is far more subject to influences beyond its own control than is likely to be the case for CPU software. Such external influences may include, in no particular order,

- the width and number of available compute units,
• the amount of available on-chip buffer memory,
• the speed of various access patterns to on- and off-chip memory,
• the ratio of available memory bandwidth to compute bandwidth,
• the latency and bandwidth between the host (CPU) and the device (GPU), and
• the instruction scheduling details of the processor in use.

Section 2 explained that GPUs are aimed at computations of a ‘streaming’ nature. It is therefore appropriate to visualize a computation running on a GPU as a network of “streams” with varying throughputs, connected to buffer spaces and processing elements that turn inputs into results in certain batch sizes. The goal of designing GPU algorithms is to first map the desired computation (e.g. matrix multiplication) onto such a network of streams, and, simultaneously, to find a mapping from these streams, buffers, and processing elements to the physically available hardware. From this picture, it becomes apparent that every nontrivial piece of GPU software represents a complicated tradeoff. In many cases, the programmer making these tradeoffs has incomplete information on the factors involved. For example, design details of the compute device may be unavailable to the programmer. But even if they are, program execution in massively parallel processors is a complicated and non-local process that may defy easy comprehension even by the processor’s designers.

GPU programming therefore relies extensively on experimentation and microbenchmarking to overcome missing knowledge of causes by obtaining measurements of symptoms. As a software developer, this is a very unsatisfying place to be in: the obtained results may not be robust to changes of hardware, problem sizes or other parameters. Further, this experimentation and benchmarking is generally tedious work that needs to be carried out systematically, consistently and repeatably. It is therefore not far-fetched to wish for these tasks to be automated. From there, it is a small step to metaprogramming, the automated reasoning about programs, and RTCG.

4. Problems Solved by GPU Run-Time Code Generation

This section is devoted to describing a number of issues that are commonly faced when programming a GPU. In each case, we point out how a GPU RTCG strategy can be used to address these issues in a natural and straightforward manner.

4.1. Automated Tuning

During the creation of a GPU program, it is natural for the programmer to come up with a number of variants of a given code, each of which will be observed to have certain properties regarding data layout and computation speed. The conventional approach to code tuning then calls for the fastest variant to survive, while the others will be discarded. This is not necessarily a desirable course of action, as information is lost. Instead, it seems more appropriate to retain as many of these variants as is practical, assuming that they hold at least some promise. Further, each variant may have a number of tunable parameters, such as loop lengths, block sizes, etc. Retaining variant information permits choosing the best one from a reasonable-size pool of candidates in an automated fashion, guided by some metric such as execution speed. This is the basic premise of automated tuning, which is trivially enabled by GPU RTCG. Further, automated tuning is not just enabled by RTCG, it is enabled at the right time—namely at run time—when complete information is available. We present three examples illustrating the type of choices optimally resolved by automatic tuning:

The first and perhaps the most important choice in GPU algorithm design is that of loop slicing, as explained in Section 2. Even loops that are trivially linear on the CPU must typically be subdivided into several levels for the GPU to be efficient, with levels corresponding to SIMD lanes, execution units, as well as serial execution. For some algorithms such as matrix multiplication, loop slicing is important even on the CPU to preserve locality of access and thereby the efficiency of on-chip caches. Since GPUs have even less
cache and even more slicing levels, getting the loop slicing right is of paramount importance to obtaining reasonable performance.

Second, many GPU architectures have user-managed on-chip memories. Upon creation of a code, it is often not obvious which pieces of data will yield the most benefit from low latency local storage. It is almost certain that on-chip memory will remain a scarce resource for the foreseeable future. Thus, peak performance necessitates tradeoffs that adapt to the hardware situation at hand.

Third, GPU architectures achieve high memory throughput not through high memory clock rates, but rather through wide data busses. Unfortunately, wide data busses only achieve acceptable net bandwidths when used to transfer large numbers of consecutive data words. Further, the bus widths are often closely matched with the widths of SIMD units in a GPU. It is to be expected that both the loop slicing of the algorithm and the layout of the data it uses will be influenced by these performance characteristics of memory access. Many strategies have been invented to deal with these restrictions, and almost all of them come with drawbacks limiting their usefulness—e.g. wasted space and SIMD lanes in the case of padding. As in the case of user-managed on-chip memory, it is desirable, but nontrivial, to choose a layout that balances advantages and disadvantages.

4.2. The Cost of Flexibility

Flexibility is commonly seen as a desirable feature of a computer code—where “code” usually means a user-facing executable. The more functions a certain executable can perform without having to be modified, the better. Yet there exists a flexibility versus performance trade off. As an example that is the polar opposite of flexibility, one may consider an optimized code that can only multiply matrices of a certain size. No matter how fast or otherwise attractive such a code may be, unless the user’s desired application requires matrix multiplications of this size, it is entirely useless. Thus almost all computer codes are built with at least some flexibility.

It should then be realized that flexibility comes at a cost: Constants get replaced by variables, formerly fixed loop trip counts become variable, and quite generally a compiler has less knowledge available at compile time, making its optimizer less effective. The process of removing such flexibility, on the other hand, is generally frowned upon and derisively called “hardcoding”. We feel, however, that this point of view has no merit once run-time code generation is available, as one is at liberty to generate code for exactly one purpose—any extra flexibility is likely just unneeded ballast.

In compile-time metaprogramming frameworks, hardcoding is sometimes replaced by generating a large number of potentially needed code variants ahead of time by considering anticipated needs for different problem sizes, data types, etc. Once the number of variants surpasses “a few”, the costs of this approach quickly become very significant both in compilation time and memory footprint of the executable. In comparison, GPU RTCG suffers no such scaling penalty: It can use information available only at run time to cut down the number of variants that need to be generated, it can use caching to amortize the cost of finding the optimal code, and unused code variants can be disposed of immediately.

4.3. High-Performance Abstractions

Nearly all computer programs are built in ‘layers’, where each individual layer solves a certain subproblem and presents a more abstract, ‘higher-level’ interface to surrounding layers. This is good engineering practice, as it allows partitioning a big problem into many smaller ones, and it enables reuse of engineering effort. In some cases, this layering is easily achieved and results in very little loss for the ‘consumer’ of the interface. In other cases, such abstractions can be made uneconomical by coding circumstance. We will first look at examples of how this might happen, and then at what RTCG does to improve the situation. One common instance of uneconomical abstractions occurs when a consumer of an interface needs to specify details about an operation that is to be performed on large volumes of data, as part of an inner loop in the abstraction. As a trivial example, consider an abstract form of vector addition allowing a variety of scalar types.

An easy (but unsuitable) run-time technique is the use of function pointers (or equivalently, virtual methods). In the frame of our example, each scalar addition under this scheme would require a computed call to a subroutine carrying out the addition on the scalar level. While this allows the required level of
run-time polymorphism, it is very expensive: A floating point addition can usually be carried out in a single machine clock cycle, but a computed jump may defeat prediction logic, stall the execution pipeline, and can easily take several orders of magnitude longer than the operation it is meant to perform. Furthermore, the requisite computed calls are unavailable on many types of GPUs.

The disadvantages of the function pointer approach drove the development of mechanisms for compile-time polymorphism on the CPU and the GPU. In C++, this is achieved through the use of class and function templates. If the user’s customization is assumed to be known at compile time, the compiler can make use of that knowledge and generate efficient code. In our example, the vector addition would be written with respect to an unspecified type, relying (for example) on the assumption that the underlying scalar supplies addition. The type of the scalar is required to be known at compile time, and hence the compiler can statically find the addition routine and substitute (“inline”) its use, ideally eliminating all overhead. This is a popular approach, but it has two shortcomings: First, it requires early concretization. In the example, all desired uses of the vector addition code have to be known before the program is run. Second, the C++ template mechanism in particular responds unfavorably to complexity growth. It makes simple things like type substitution quite easy. But templates alone, even without the rest of C++, form a fully capable—if awkward—programming language [39], and some implementers have seen this as an invitation to do rather advanced things with them. While such use validates the need for a meta-level where code is able to reason about other code, the actual end results in this case tend to be both brittle and complicated.

The ideal solution would be a compromise of these two. Function pointers are simple, flexible and do not require early concretization, while templates have very little overhead. By removing the distinction between ‘compile time’ and ‘run time’, RTCG fills this void. Once RTCG is available, appropriate code can be generated whenever a different requirement arises, leading to flexibility. RTCG code is also fast—it can do away with any sort of flexibility, because it can safely be considered “single-purpose”. Further, code generation can be seen as a text processing task. Since one is not limited in the choice of tools with which to perform this generation, RTCG-based codes can be as simple as possible and respond favorably to complexity growth.

4.4. GPUs and the Need for Flexibility

As a final comment, it should be emphasized that in the past, due to the associated development complexity especially for C++-based techniques, metaprogramming was restricted to high-need applications. The cost of metaprogramming outweighed the disadvantages of “hardcoding” only for the largest of projects.

GPUs however democratize this need, as they put a larger penalty on inflexible, untuned code. By deciding to perform a GPU port of an algorithm, one implicitly states that one is willing to trade some implementation effort for a substantial performance gain. As explained above, finding a good implementation is often nontrivial, and therefore the potential gain from RTCG is large. In other words, GPUs increase the relative cost of not using metaprogramming techniques, and therefore it is likely that code generation and techniques like it will see much wider adoption. However, good tools are required to allow the broadest possible cross-section of developers to take advantage of RTCG.

5. PyCUDA: A Scripting-Based Approach to GPU RTCG

We have seen in the previous section that GPU RTCG solves a number of pressing problems in the development of high-performance compute-oriented codes. In this section, we present PyCUDA, a practical and mature open-source toolkit supporting GPU RTCG.

While its name already suggests that PyCUDA connects the high-level Python programming language [38] with the Nvidia CUDA compute abstraction [27], at least the first choice deserves justification. The major factor in choosing a high-level, dynamic programming language over a potentially better-performing, low-level, static one is the complementarity of tasks between the GPU and the host processor. The GPU is optimally suited to carrying out throughput-oriented parts of a program, namely the part that would have conventionally constituted the ‘inner loops’. Freed from this duty, the CPU now is responsible for “only” control and communication (including, e.g., disk input/output). In other words, it now works at
a higher level of abstraction. Therefore a high-level scripting language (such as Python) can perform this higher-level job equally well or better, simply because the performance demands are reduced, and both code generation and execution control can be of considerable complexity. Control input is needed by the GPU about once every millisecond, and code generation is needed even less frequently. A Python-based GPU compute code will have no trouble realizing the same full performance potential of GPU hardware as a C-controlled GPU compute code, but with much less effort on the part of the programmer. This reduction in effort is achieved in many ways—for example, data types and resources are managed by the language itself instead of by a human, also closures and other high-level constructs are available. Relatedly we would like to emphasize that PyCUDA does not inhabit Python’s software ecosystem by itself: a large number of packages for such diverse purposes as plotting, computer algebra, or optimization are available easily and under liberal licenses [20]. Significantly, the mpi4py package [6] in conjunction with PyCUDA allows a straightforward combination of shared-memory GPU-based and distributed-memory MPI-based parallelism. The easy availability of a multitude of packages contributes to making scripting languages more productive than their conventional compiled counterparts. Scripting languages such as Python or even MATLAB are already popular for exploratory prototyping, but in combination with a GPU, their usefulness extends well into the territory of ‘full-scale’ codes.

PyCUDA itself is built from multiple levels. At the lowest level, PyCUDA makes the entirety of the CUDA run-time system available from Python by introducing a thin object-oriented shell. In this context, we would like to emphasize the word “entirety”: Every feature of the CUDA run-time system is accessible from Python via PyCUDA, including textures, pinned host memory, OpenGL interaction, zero-copy host memory mapping, etc.

While this low-level interface translation is relatively straightforward, care was taken to make the interface a “good citizen” of the high-level-language system: Memory allocation and resource management concerns are handled automatically in close coordination with the Python garbage collector, avoiding spurious resource shortages. Entities such as textures, code modules, and compute devices are reflected into Python using object-oriented terms, providing better abstraction than the low-level C interface. Errors are detected and reported automatically. Further, programmers of high-level languages expect that their programs do not abort upon executing erroneous code, that most error conditions are recoverable and that useful feedback is available on what happened that caused the error. PyCUDA satisfies these expectations. Care is taken however that these automatisms do not turn into a liability. For example, a program under tight memory constraints may not have the luxury of allowing automatic resource management. For this use case, PyCUDA still allows the user to manually control deallocation of resources.

Figure 2. Workflow of PyCUDA GPU program compilation. PyCUDA aims to maintain a scripting-like “edit-run-repeat” style of working for the user. The compilation and caching operations in the gray box are performed without user involvement.

The basic shell described so far establishes the basis for more interesting, higher-level features. PyCUDA augments the runtime system by a critical capability: It allows the user to easily create on-GPU binaries.
simply by providing C-like CUDA source code as a simple character string. This capability is what enables GPU run-time code generation.

Two factors contribute to making this process easy and transparent: First, the user makes no contact with the underlying CUDA compiler infrastructure unless desired. Second, the result of the compilation process is stored in a semi-permanent cache and reused if possible. The cache is sensitive to changes in the hardware and software environment and initiates recompilation when necessary. As a result, compilation of source code and subsequent loading of the binary code becomes nearly instantaneous and invisible to the user, and the quick turn-around time of a scripting-based programming environment is retained. Figure 2 illustrates the principle, the end result of which is to make computations specified by C source code a library service that is available cheaply.

Further, whenever GPU RTCG is used for automated tuning, it is desirable that the expense of time and processing power involved in the tuning is only incurred once per relevant code change. In most cases, the presence of a compiler cache is already sufficient here, as compilation is usually several orders of magnitude more time-consuming than the actual timing run of the code. However, when that is not the case, PyCUDA supports the building of an application-level cache by offering means for the easy gathering of identifying information regarding hardware, software and their corresponding versions.

The combination of RTCG with services of the run-time system such as high-precision timing and code property access already suffices to enable the strategies laid out in Section 4. Figure 3a illustrates, by way of a sample program, how the pieces of PyCUDA explained so far fit together.

5.1. Abstractions in PyCUDA

One of the fundamental principles in PyCUDA is that while high-level features are desired, their use should never obstruct access to low-level features, and their use should never obscure the underlying processes. The purpose of this is twofold:

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Figure 3. a) An example of the use of PyCUDA, showing the use of the SourceModule facility for (static) GPU run-time code generation. This simple program uploads a 4 x 4 array of single-precision floating point numbers, multiplies them by two on the GPU, and retrieves the result. b) An example performing the same function as a), but using GPUArrays.

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For completeness, it should be mentioned that PyCUDA also allows the just-in-time compilation of code expressed in Nvidia's lower-level "PTX" abstract machine language.
• Uninhibited low-level access ensures that all opportunities for unanticipated uses of low-level facilities are retained.

• Whenever a high-level abstraction is used, the developer deciding to use it assumes a responsibility to know what the abstraction does, fix it if it breaks, or adapt it if it is no longer suitable.

Keeping this in mind, PyCUDA does include a number of abstractions, but strives to keep them simple and “flat”. It further strives to only include “popular” abstractions that are expected to be useful to a significant share of client codes, lessening the maintenance burden on every individual user.

5.1.1. PyCUDA GPU Arrays

PyCUDA provides computational linear algebra involving vectors and multi-dimensional arrays that are designed to match the interface of the widely-used (CPU-based) Python array package numpy [28]. This array class, called GPUArray, offers a complete set of features, including

• elementwise algebraic operations such as addition, multiplication, etc.,

• a full set of floating-point transcendental as well as utility functions,

• type promotion and arbitrary combinations of data types (e.g. adding 32-bit integers to 32-bit floating point values results in 64-bit floating point values to preserve precision),

• reductions such as sums, maxima, and inner products, and

• tight integration with the numpy [28] Python array package.

Using the GPUArray infrastructure, PyCUDA also implements GPU-based sparse matrix-vector multiplication, as described by Garland and Bell [1, 2]. Based on this feature, in turn, we were able to include a fast conjugate-gradient-based [13] linear system solver, which uses the GPU to solve large systems about ten times faster than competing CPU implementations. Both of these facilities interact seamlessly with the CPU-based SciPy module [15].

a)

```python
import pycuda.autoinit
import pycuda.gpuarray as gpuarray
from pycuda.curandom import rand as curand
from pycuda.elementwise import ElementwiseKernel

x = curand((500000,))
y = curand((500000,))
z = gpuarray.empty_like(x)

lin_comb = ElementwiseKernel(
    "float a, float *x, float b, float *y, float *z",
    "z[i] = a*x[i] + b*y[i]"
)(5, x, 6, y, z)
```

b)

```python
import pycuda.autoinit
import pycuda.gpuarray as gpuarray
from pycuda.curandom import rand as curand
from pycuda.elementwise import ElementwiseKernel, \VectorArg, ScalarArg

x = curand((500000,))
y = curand((500000,))
z = gpuarray.empty_like(x)

lin_comb = ElementwiseKernel([\ ScalarArg(x.dtype, "a"), VectorArg(x.dtype, "x"), \ScalarArg(y.dtype, "b"), VectorArg(y.dtype, "y"), \VectorArg(x.dtype, "z")], 
    "z[i] = a*x[i] + b*y[i]"
)(5, x, 6, y, z)
```

Figure 4. Elementwise linear combinations implemented via PyCUDA’s elementwise-operation code generator, accessible as pycuda.elementwise.ElementwiseKernel. a) shows a simple, statically typed version. b) shows a version that relies on type introspection to generate code that is appropriate for the given combination of array types. (The result type is defaulted to the first argument’s type for simplicity.)

On top of GPUArrays, PyCUDA offers code generation features for custom elementwise and reduction operations. These work by letting the user specify only short snippets of C code for core functionality, while
supplying loop slicing and driver code automatically. Figure 4a) illustrates this for the elementwise operation case, implementing a two-vector linear combination. The reduction code generator is similar in spirit. We would like to emphasize the ease with which this simple RTCG tool overcomes the common problem of proliferation of temporary variables plaguing abstract, operator-overloading array packages. C++ packages employing template techniques can achieve a similar degree of efficiency through the expression template mechanism [40], but a robust, usable implementation of this technique is far more complex than the simple generation of C code involved in the RTCG solution. In general, the effort required to create RTCG programs scales very gently with the degree of sophistication required. Figure 4b) illustrates this by extending the previous linear combination code to adapt the vector types in the generated code dynamically, by making use of Python’s run-time type introspection. It may be argued that these examples look pleasant only because PyCUDA contains a nice enough pre-made user interface that suits this purpose. This is certainly true, but this should be seen in a different light: Only by working in a high-level language were we able to provide this type of user interface. Since providing usable, abstract interfaces is more straightforward in scripting environments, this niceness becomes the rule rather than the exception.

5.2. Code Generation with PyCUDA

We now turn to how a user might go about creating abstractions such as ElementwiseKernel herself. Since PyCUDA can natively process C code (or rather CUDA’s flavor thereof), the objective is the generation of such code. PyCUDA makes no assumptions about the origins of the code it processes, which allows the logic involved in the generation to be designed to match the needs of the application. There are, however, three suggested ways of generating code which we have found to cover a variety of needs.

a) from jinja2 import Template
tpl = Template(""
  @global_ void add(
    {{ type_name }}* tgt,
    {{ type_name }}* op1,
    {{ type_name }}* op2)
  {
    int idx = threadIdx.x +
      {{ thread_block_size }} * {{ block_size }}
    * blockIdx.x;
    {% for i in range( block_size ) %}
      tgt[idx + {{ offset }}] =
        op1[idx + {{ offset }}] + op2[idx + {{ offset }}];
    {% endfor %}
  }"")
rendered_tpl = tpl.render(
  type_name="float", block_size=block_size,
  thread_block_size=thread_block_size)
smod = SourceModule(rendered_tpl)

b) from codepy.cgen import FunctionBody, 
  FunctionDeclaration, Typedef, POD, Value, 
  Pointers, Module, Block, Initializer, Assign
from codepy.cgen.cuda import CudaGlobal
mod = Module([
  FunctionBody(
    CudaGlobal(FunctionDeclaration(
      Value("void", "add"),
      arg_decls=[Pointer(POD(dtype, name))
              for name in ["tgt", "op1", "op2"]]),
    Block(
      Initializer (   POD(numpy.int32, "idx"),
        "threadIdx.x + %d*blockIdx.x"),
      % (thread_block_size * block_size)),
      )]
    )]
  )]
mod = SourceModule(mod)

Figure 5. Different methods of Run-Time Code Generation (RTCG) with PyCUDA. Example a) generates a piece of C code from a textual template implementing an unrolled version of vector addition. (using the Jinja2 engine [33] in this instance) Example b) builds a data structure approximating a C syntax tree for the same purpose as a). This tree is then converted to C code using the authors’ codepy package [17]. Full context for both examples can be found in the PyCUDA source tree as examples/demo_meta_template.py and examples/demo_meta_codepy.py.
Simple textual keyword replacement. This simple technique performs the equivalent of search-and-replace on source code. It suffices for a surprisingly large range of use cases, such as the substitution of types and constants into source code at run time. Its technological reach is increased by combining it with C preprocessor macros. Further contributing to its attractiveness, Python’s standard library can perform keyword substitution without relying on external software.

Textual Templating. For code generation applications where control flow and conditionals are required, but all code variants are textually related, the use of a so-called templating engine, commonly used for the generation of web pages, offers a natural escalation of the capabilities of keyword substitution. Many templating engines (and correspondingly, templating languages) exist. Figure 5a) demonstrates the use of the Jinja2 [33] engine for the generation of a simple, partially unrolled vector addition code.

Syntax Tree Building. The use of templating finds its limits if the codes to be generated cease to be textually related. Then it becomes appropriate to introduce a full representation of the target code in the host language. The most general such representation is in the form of a syntax tree. Syntax tree building allows code to be generated using all facilities of the host language. In particular, while templating is mostly “flat” and oriented along the lines of the output, syntax tree building allows the user to use, e.g., a hierarchy of functions to generate the desired code.

Figure 5b) demonstrates the use of the authors’ CodePy [17] package for the generation of the same unrolled vector addition code as in the previous example. Comparing Figures 5a) and b) also reveals that syntax tree generation does not represent a “giant leap” when compared to templating. This again serves to emphasize the gentle growth of complexity in GPU RTCG with PyCUDA.

We have already emphasized various times that one of the central goals of PyCUDA is to facilitate the construction of abstractions, the more sophisticated of which amount to domain-specific languages. From a compiler construction perspective, the three strategies above amount to using C as an intermediate representation in the building of a compiler for such a language. Given that PyCUDA is not aimed at optimization at the lowest, machine-language levels, this seems to be an appropriate choice.

PyCUDA is available from http://mathema.tician.de/software/pycuda under the liberal MIT open-source software license. Full documentation is available online and packaged with the distribution, along with a large body of examples and tests. The package supports all platforms on which CUDA is available. PyCUDA has been used in a variety of research codes (see Section 6 for a few examples). In addition, PyCUDA can be used interactively from the command line as well as from the notebook interface of the Sage exploratory computation system [35].

5.3. PyOpenCL: OpenCL and GPU RTCG

For those concerned about the vendor specificity of the CUDA compute abstraction, PyOpenCL, a sister project of PyCUDA, has recently been released by the authors under the same terms and is available from http://mathema.tician.de/software/pyopencl. It targets the OpenCL [12] industry standard compute abstraction. PyOpenCL extends the methods presented thus far to a significantly wider range of devices and vendors. At the time of this writing, PyOpenCL enables the basic premise of this paper, but has not yet grown to include most of the high-level facilities available in PyCUDA.

6. Successful Applications

PyCUDA has been used successfully in a considerable number of research projects. We outline a few projects and their use of RTCG in detail below. Beyond those, the following researchers have agreed to let us mention their use of PyCUDA:

- Ian Cullinan and the SAFE Advanced Surveillance group at NICTA are using PyCUDA to search large facial image databases. Their work seamlessly integrates a GPU-accelerated search algorithm with a Python web interface written using the Django framework. Using PyCUDA for this task approximately halved the time it takes to run a search.
6.1. Discontinuous Galerkin Finite Element PDE Solvers

Discontinuous Galerkin finite element methods (DG-FEM) for the numerical solution of partial differential equations are popular because they are both flexible and robust: They allow arbitrary geometries and easy control of accuracy without compromising simulation stability. In addition to their favorable numerical properties, DG schemes combine high arithmetic intensity, local memory access and locally dense linear algebra. They are therefore computationally well-suited for implementation on GPUs. However, DG-FEM also face significant challenges for GPU implementation, many of which were already captured in abstract form above. For example, DG uses data sizes that are not usually powers of two. Its data reuse pattern could benefit from more on-chip memory than is currently available, so a fetch schedule must be chosen carefully. And finally, loop slicing can have a significant impact. When exploring loop slicing, we have found an up-to-date listing of successful uses of PyCUDA, PyOpenCL and GPU run-time code generation in general can be found on the web at [http://wiki.tiker.net/PyCuda/ShowCase](http://wiki.tiker.net/PyCuda/ShowCase).

- Tomasz Rybak at Bialystok Technical University is applying GPU computing to the generation of recurrence diagrams for time series analysis. Using PyCUDA for his analyses, he was able to achieve an 85-fold speedup of his computations. He is using code generation strategies to achieve even greater speeds in cases when data set characteristics allows for using faster memory.

- Chris Heuser with the Center for the Study of Complex Systems at the University of Michigan used PyCUDA to implement an agent-based model. PyCUDA allowed for the easy integration of many of the model’s features. In the future, RTCG will be used to allow run-time alterations of agent characteristics, world size, and other model parameters.

- Romain Brette and Dan Goodman are using PyCUDA to simulate spiking neural networks with their simulator “Brian” [11]. Brian relies on PyCUDA to generate run-time GPU code for the integration of differential equations provided by the user in a Python script. GPU performance was up to 60 times faster than a comparable CPU implementation for some models.

An up-to-date listing of successful uses of PyCUDA, PyOpenCL and GPU run-time code generation in general can be found on the web at [http://wiki.tiker.net/PyCuda/ShowCase](http://wiki.tiker.net/PyCuda/ShowCase).

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**Figure 6.** a) A sample scattering problem solved using the DG-FEM methods described Section 6.1. The incident plane-wave electric field is shown as pseudocolor values on the scatterer, while the scattered electric field is shown as arrows. The computation was performed at fourth order on a mesh of 78745 elements using an incident-field formulation [14] and characteristic absorbing boundary conditions. It achieved and sustained more than 160 GFlops/s using a single Tesla C1060. b) A schematic diagram of the family of biologically-inspired computer vision models considered in Section 6.2. The system architecture consists of three feedforward filtering layers, with the filters in each layer being applied across the previous layer. Red colored labels indicate a selection of configurable parameters (only a subset of the 52 parameters are shown). Exploring this family efficiently was fundamentally enabled by the methods and tools described in this paper, as writing optimal GPU code for any model instantiation by hand would be prohibitive.
it advantageous to consider not only the conventional execution-in-sequence and execution-in-parallel, but also a third, mixed (“inline-parallel”) form where independent results are computed within one execution context. This sometimes helps to extract further reuse from data already loaded into registers.

An outline of the methods we have developed to bring DG onto the GPU was recently published [18]. In addition, we find that DG responds almost ideally to the RTCG techniques described above. We employ an automated tuning procedure relying on code generation using CodePy. The first (or “outermost”) tuning stage concerns memory layouts. A number of layouts are tried with subsequent stages. For each given memory layout, we exploit that DG operators can be split into a number of independent operations, each of which is then tuned independently, using various choices for, e.g. loop slicing and use of on-chip storage. From these individual measurements, a joint score assigned based on a target operator, and the memory layout is chosen based on this score. While the procedure is still mainly brute-force in nature, it employs a few heuristics to recognize poor solutions early on. The object of interest here is a solver for Maxwell’s equations on a general 3D unstructured grid. We found that for high orders of accuracy, numerous fast code variants exist, and manual tuning is feasible (if tedious), while at lower orders, fast codes seem to be less abundant and depend on “lucky coincidences” that are difficult to find by hand. This difficulty is owed in part to many of the matrices’ sizes being ill-suited to the number of SIMD lanes available. By combining a few techniques aimed specifically at low orders with high-order optimizations found by a colleague through hand-tuning, we were able to create a code that auto-tunes itself to automatically work well across a large range of orders. At order three, it achieves 138 GFlops/s using a single Nvidia GTX280 GPU. Performance then increases rapidly (and smoothly) until it plateaus well above 200 GFlops/s at orders five and above. (A. Klöckner, T. Warburton)

6.2. Computational Visual Neuroscience

The study of biological vision and the creation of artificial vision systems are naturally intertwined as they represent simultaneous efforts to forward and reverse engineer systems with similar goals. However, while neuroscience has provided inspiration for some of the “broad-stroke” properties of the visual system, much is still unknown. To pave a way forward, we have developed a high-throughput approach [30] to more expansively explore the possible range of brain-inspired models (Figure 6b), including models of larger, more realistic scale, leveraging recent advances in commodity stream processing hardware. In analogy to high-throughput screening approaches in molecular biology, we generate and train thousands of potential model instantiations, and “screen” their visual representations using an object recognition task. From these candidate models, the most promising are selected for further analysis. We have shown that this approach can yield significant, reproducible gains in performance across an array of basic object recognition tasks, consistently outperforming a variety of state-of-the-art purpose-built vision systems from the literature, and that it can offer insight into which computational ideas are most important for achieving this performance.

The brain itself is a highly parallel statistical supercomputer, and thus algorithms inspired by its function are well suited to the computational advantages offered by GPUs. However, this power naturally comes at the cost of increased complexity for the developer (Section 4). In the last three years, we have experienced three different paradigms (i.e. programming GPUs with graphics primitives in 2006, programming the PlayStation 3 using low-level Cell intrinsics in 2007 and programming GPUs with compute primitives in 2008). To overcome the challenge of optimizing each architecture, we applied RTCG to auto-tune the core operations by instrumentalizing low-level code and manipulating it with a Python template engine (Figure 5b). We implemented common optimization strategies (e.g. loop unrolling [16], pre-fetching and software pipelining [19], alleviation of register pressure using spilling [42], communication and computation load distribution, etc.) and achieved comfortable speed-ups with a simple auto-tuning method (i.e. random search on a coarse grid). In the future, we plan to investigate the use of machine learning techniques for auto-tuning, an approach recently undertaken by IBM’s Milepost GCC [10].

Using RTCG toolkits like PyCUDA, we were thus able to combine the flexibility and ease-of-use of a high-level language for “outer loop” control and auto-tuning, with the raw performance of highly optimized “close-to-the-metal” GPU or Cell code to achieve hundred-fold speedups over conventional MATLAB/MEX CPU implementations (the standard in the fields of computational neuroscience and computer vision; see
We argue that the combination of these qualities enables a new kind of exploration of ideas in biological and computational vision, where scale is matched with the fluid ability to experiment with new ideas.

As the scale of available computational power continues to expand, and more RTCG tools like PyCUDA emerge, we believe that this approach has the potential to greatly accelerate progress in both artificial vision and our understanding of the computational underpinning of biological vision. (N. Pinto)

### 6.3. Selective Embedded Just In Time Specialization

We have also used PyCUDA as the foundation of higher level programming tools, performing Selective Embedded Just In Time Specialization [3]. The idea behind SEJITS is to provide highly productive environments for parallel programming through the use of specialized runtime code-generation. We create domain specific modules, called specializers, which use metaprogramming to analyze a high level description of a particular computation, and then perform JIT code generation for that particular computation. In this case, we express our computations in Python, and use Python function decorators to intercept procedure calls which should be specialized. Python’s introspection facilities allow us access to the source of a procedure under specialization, which we then analyze and manipulate to generate CUDA source code. Using PyCUDA, we move data back and forth between the Python interpreter and the GPU, as well as execute the specialized CUDA code.

![Selective Embedded Just-In-Time Specialization](image)

Figure 7. Selective Embedded Just-In-Time Specialization

Figure 7 outlines this approach. Because the specialization machinery and the domain specific modules are embedded in a scripting language, it is easy for programmers who understand efficient implementation to incrementally add specializers for new domain abstractions, which then can be exported for use by those less familiar with the details of efficient parallel implementation. Additionally, embedding the code to be specialized in a scripting language allows us to fall back to execution by the high-level interpreter, if a particular idiom is not supported by a specializer. Finally, SEJITS allows for the incorporation of autotuners to generate multiple variations of a particular computation, which is very useful when attempting to provide good performance on diverse target architectures.

We prototyped a set of specializers for image processing applications, providing some abstract stencil and category reduction primitives to allow the implementation of image processing routines including k-means clustering and edge detection, taken from a high-end image contour detection algorithm [4]. On simpler types of code, such as image convolution, our SEJITS system ran only about 3x slower than our hand-optimized convolution routines. Due to naive code-generation in our specializers, on more complicated types of code, such as the k-means clustering routines, our system was about 10x slower than hand-optimized CUDA code, although we believe the code generators can still be substantially improved, which is ongoing work. In summary, RTCG with PyCUDA has enabled research into higher-level programming models and compilers for parallel platforms, by bridging the gap between a high-level language, Python, and a highly-parallel platform, the GPU. (Y. Lee and B. Catanzaro)
6.4. Estimating the Entropy of Natural Scenes

Characterizing the statistics of natural scenes is an important area of vision research. The entropy of images provides a measure of the information content available to the visual system and as such quantifies the demands placed on neural information processing mechanisms. From an applications perspective, entropy is the theoretical limit of compression—the lower bound on any compression scheme. Recently, [5] used an entropy estimation algorithm to binlessly estimate the entropy of small patches of natural images from the distribution of nearest-neighbor (NN) distances. This approach is limited by requiring NN calculations of an exponentially growing set. We overcome this limitation by porting the parallel brute force NN search to the GPU. This enables us to perform more extensive entropy and fractal dimensionality analyses on the entire database of about 4000 thousand natural images, only a few dozen of which were used in for the previous work [37]. One 8800GTX card performs 30 times faster than a compiler optimized C version, 53 times faster on a GTX 295. Additionally, because our implementation uses PyCUDA, we can easily optimize the parameters of the implementation for newer cards, and extend the parallelism to multiple cards. Such computational capabilities will enable us to analyze and compare previously unimaginable large classes of images in a reasonable amount of time. (P. Ivanov)

6.5. Filtered Backprojection for Radar Imaging

Tomographic systems as diverse as x-ray CT and synthetic aperture radar all use a sensor that projects a three-dimensional function (such as x-ray absorption and electromagnetic reflectivity, respectively) onto one-dimensional range profiles. Reconstruction of the original function from a collection of these line projections can be accomplished by the filtered backprojection algorithm, where each voxel must query each line projection for its contribution to that voxel, which can be done in $O(N^3)$ time. Leveraging the large number of cores and the linear interpolation hardware available on modern GPUs, a mildly-optimized CUDA implementation performs SAR backprojection over 50 times faster on a C1060 Tesla than a single-threaded implementation on a modern CPU. Anecdotes about hyperoptimized industrial implementations support the quality of this comparison where, e.g., a Tesla implementation is claimed to be roughly 10 times faster than a multi-threaded 4-core Intel Xeon implementation.

An all-C CUDA implementation can either have a kernel that can accept several arguments for radar- and geometry-specific parameters, or these parameters can be pre-compiled as constants. The latter increases the conciseness of the kernel code, but requires separate binary executables for different imaging scenarios—and neither precludes the risk of errors in programmer-controlled memory management. PyCUDA makes it trivial to automatically generate kernels with pre-compiled constants, allowing the CUDA kernels to be much simpler. This also allows the experimentation that is inherent in tuning a CUDA implementation to be done rapidly in a command-line environment. Thus, in our experience, both these advantages combine to dramatically decrease both code size and tuning time when using PyCUDA. (A. Fasih)

7. Conclusions

We have described the powerful consequences of the confluence of two events in high-performance computing: First, the emergence of general-purpose programmable GPUs as a viable mass market product has made performance jumps of an order of magnitude or more a reality for a number of important applications. Second, the maturing of open-source scripting languages and their software ecosystems has enabled similar jumps in productivity for creators of scientific software. It is straightforward to see that a hybrid model combining GPUs and scripting offers numerous advantages over more traditional models of software creation.

The main message of this paper is that through the natural addition of GPU run-time code generation to this mixture, one automatically combines the strengths and compensates for the weaknesses of each of the technologies involved, leading to a compelling way of constructing high-performance computational software.

To make GPU RTCG accessible, we have built, documented, and published PyCUDA, a toolkit that allows the easy application of the principles described here. We have described the facilities available in PyCUDA and demonstrated their use. We will continue to extend and maintain both PyCUDA and PyOpenCL.
Based on these toolkits, we will explore the construction of tools that allow researchers to focus on their target areas, while leaving the detailed work involved in accomplishing basic computational tasks to the machine. One effort that is currently underway will use empirical optimization to try and find well-performing kernels for a certain set of basic array operations, such as those involved in dense numerical linear algebra or certain PDE solvers. Further, it should not be forgotten that PyCUDA was born out of the need of actual applications, as Section 6 illustrated. As the research in these application areas progresses, we fully expect that more advanced needs will drive the implementation of even better tools.

In summary, we believe that the flexibility of run-time generated code provides a crucial tool in unlocking the performance capabilities of advanced hardware to a broader mass of developers, and we look forward to the opportunities and challenges that future hardware generations will bring.

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